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6-Chloro-7-methyl-4-oxo-4*H*-chromene-3-carbaldehyde

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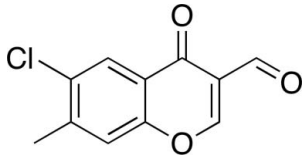
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.094; data-to-parameter ratio = 15.3.

In the title compound, $C_{11}H_7ClO_3$, a chlorinated and methylated 3-formylchromone derivative, the non-H atoms are essentially coplanar (r.m.s. deviation = 0.0670 Å), with the largest deviation from the least-squares plane [0.2349 (17) Å] being for the pyran carbonyl O atom. In the crystal, molecules are linked through π–π stacking interactions along the a axis [centroid–centroid distance between the pyran rings = 3.824 (6) Å] and two stacks are connected by type I halogen–halogen interactions between the Cl atoms [Cl···Cl = 3.397 (3) Å].

Related literature

For related structures, see: Ishikawa & Motohashi (2013); Ishikawa (2014). For halogen bonding, see: Auffinger *et al.* (2004); Metrangolo *et al.* (2005); Wilcken *et al.* (2013); Sirimulla *et al.* (2013). For halogen–halogen interactions, see: Metrangolo & Resnati (2014); Mukherjee & Desiraju (2014).



Experimental

Crystal data

$C_{11}H_7ClO_3$ M_r = 222.63
Triclinic, $P\overline{1}$
a = 3.824 (6) Å
b = 6.111 (9) Å
c = 19.962 (10) Å
α = 81.83 (7)°
β = 88.82 (7)°
γ = 87.04 (12)°
V = 461.1 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.39 mm^{-1}
T = 100 K
0.45 × 0.20 × 0.10 mm

Data collection

Rigaku AFC-7R diffractometer
2677 measured reflections
2092 independent reflections
1784 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.076
3 standard reflections every 150 reflections
intensity decay: −0.3%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.094
S = 1.08
2092 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Data collection: *WinAFC Diffractometer Control Software* (Rigaku, 1999); cell refinement: *WinAFC Diffractometer Control Software*; data reduction: *WinAFC Diffractometer Control Software*; program(s) used to solve structure: *SIR2008* (Burla *et al.*, 2007); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2010); software used to prepare material for publication: *CrystalStructure*.

The University of Shizuoka is acknowledged for instrumental support.

Supporting information for this paper is available from the IUCr electronic archives (Reference: TK5320).

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supporting information

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6-Chloro-7-methyl-4-oxo-4*H*-chromene-3-carbaldehyde

Yoshinobu Ishikawa

S1. Structural commentary

Halogen bonding and halogen···halogen interactions have recently attracted much attention in medicinal chemistry, chemical biology, supramolecular chemistry, and crystal engineering (Auffinger *et al.*, 2004, Metrangolo *et al.*, 2005, Wilcken *et al.*, 2013, Sirimulla *et al.*, 2013, Mukherjee & Desiraju, 2014, Metrangolo & Resnati, 2014). We have recently reported the crystal structures of halogenated 3-formylchromone derivatives 6,8-dichloro-4-oxochromene-3-carbaldehyde (Ishikawa & Motohashi, 2013) and 6-chloro-4-oxo-4*H*-chromene-3-carbaldehyde (Ishikawa, 2014). Both halogen bonding between the formyl oxygen atom and the chlorine atom at 8-position and type I halogen···halogen interaction between the chlorine atoms at 6-position are observed in 6,8-dichloro-4-oxochromene-3-carbaldehyde (Fig. 3, (top). On the other hand, a van der Waals contact between the formyl oxygen atom and the chlorine atom at 6-position is found in 6-chloro-4-oxo-4*H*-chromene-3-carbaldehyde (Fig. 3, middle). As part of our interest in these types of chemical bonding, we herein report the crystal structure of a monochlorinated and methylated 3-formylchromone derivative 6-chloro-7-methyl-4-oxo-4*H*-chromene-3-carbaldehyde. The objective of this study is to reveal the inductive effect of the vicinal electron-donating group on the chlorine atom at 6-position and its interaction mode.

The mean deviation of the least-square plane for the non-hydrogen atoms is 0.0670 Å, and the largest deviation is 0.2349 (17) Å for O3 (Fig. 1).

In the crystal, the molecules are stacked with the translation-symmetry equivalent^{i} [centroid–centroid distance between the pyran rings = 3.824 (6) Å, i: $x + 1$, y, z], as shown in Fig. 2. In addition, a type I halogen···halogen interaction is observed between the chlorine atoms at 6-position [Cl1···Cl1^{ii} = 3.397 (3) Å, C5–Cl1–Cl1^{ii} = 148.41 (7)°, ii: $-x$, $-y$, $-z$], as shown in Fig. 3 (bottom). Thus, a contact between the formyl oxygen atom and the chlorine atom at 6-position is not observed in the title compound. The chemical nature of the chlorine atom at 6-position in the title compound should be similar to that of the chlorine one at 6-position in 6,8-dichloro-4-oxochromene-3-carbaldehyde.

S2. Synthesis and crystallization

Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an acetonitrile solution of the commercially available title compound at room temperature.

S3. Refinement

The C(sp^2)-bound hydrogen atoms were placed in geometrical positions [C—H 0.95 Å, U_{iso}(H) = 1.2U_{eq}(C)], and refined using a riding model. One reflection (0 0 20) was omitted because of systematic error.

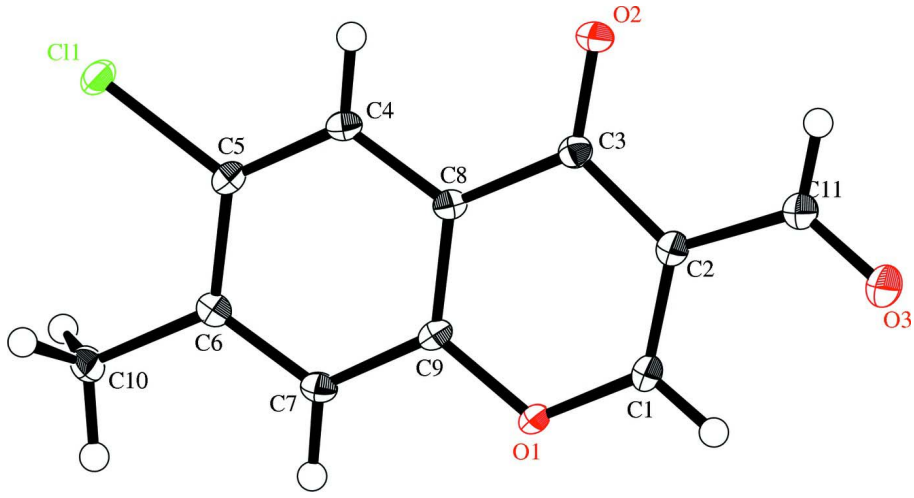

Figure 1

The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level. Hydrogen atoms are shown as small spheres of arbitrary radius.

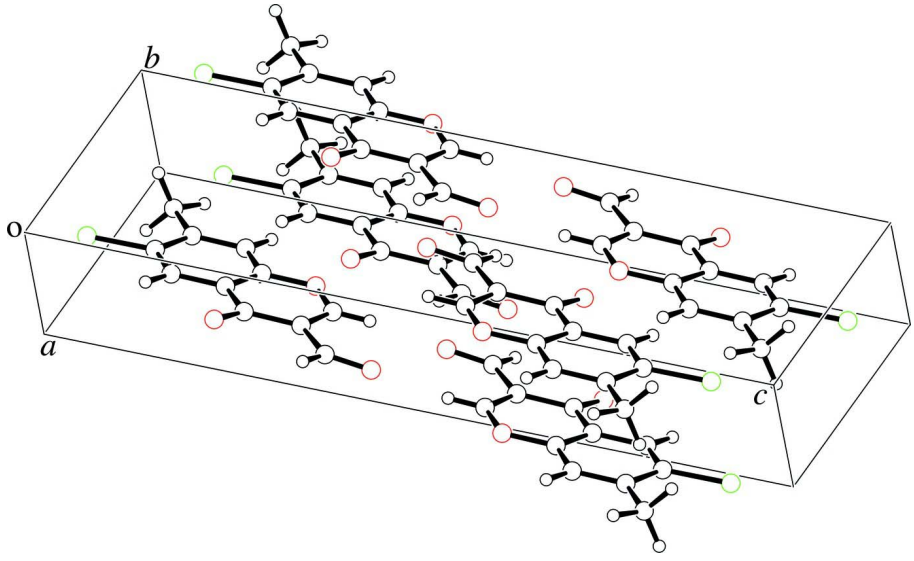

Figure 2

A packing view of the title compound.

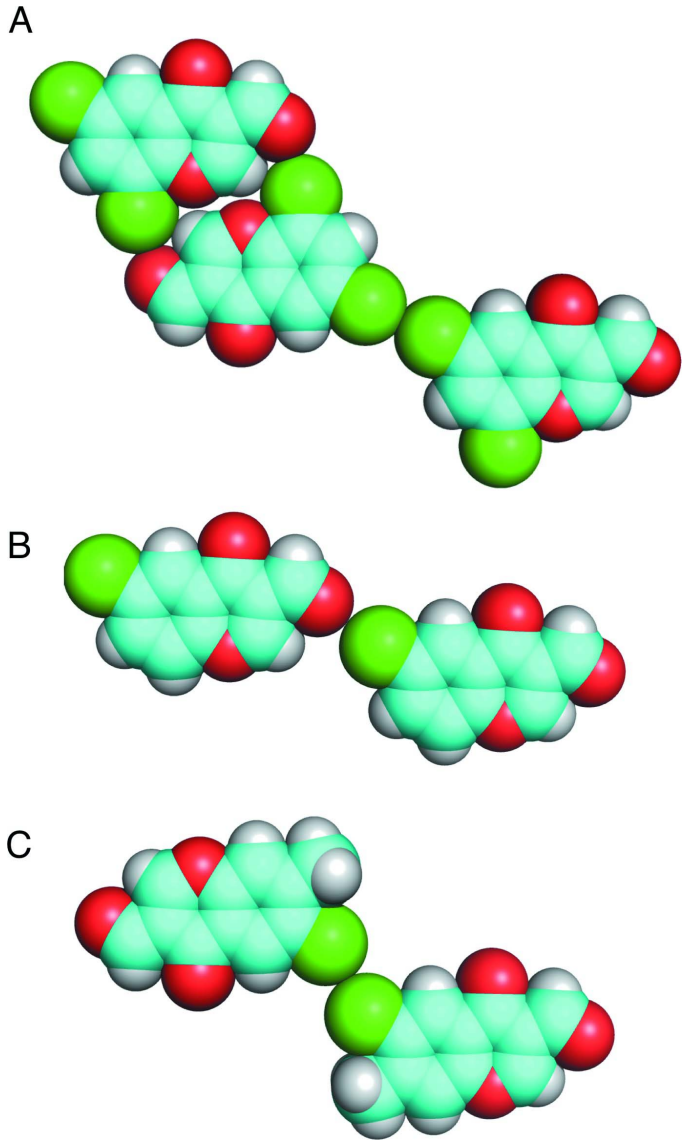

Figure 3

Sphere models of the crystal structures of 6,8-dichloro-4-oxochromene-3-carbaldehyde (top), 6-chloro-4-oxo-4*H*-chromene-3-carbaldehyde (middle), and the title compound (bottom).

6-Chloro-7-methyl-4-oxo-4*H*-chromene-3-carbaldehyde

Crystal data

$C_{11}H_7ClO_3$
$M_r = 222.63$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 3.824\ (6)$ Å
$b = 6.111\ (9)$ Å
$c = 19.962\ (10)$ Å
$\alpha = 81.83\ (7)°$
$\beta = 88.82\ (7)°$
$\gamma = 87.04\ (12)°$
$V = 461.1\ (10)$ Å^3
$Z = 2$
$F(000) = 228.00$
$D_x = 1.603$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 15.1–17.5°$
$\mu = 0.39$ mm^{-1}

T = 100 K
Plate, colorless

0.45 × 0.20 × 0.10 mm

Data collection

Rigaku AFC-7R diffractometer
ω–2θ scans
2677 measured reflections
2092 independent reflections
1784 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.076

θ_{max} = 27.5°
h = −4→2
k = −7→7
l = −25→25
3 standard reflections every 150 reflections
intensity decay: −0.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.094
S = 1.08
2092 reflections
137 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 0.2265P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

Special details

Refinement. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0\ \sigma(F^2)$ is used only for calculating R-factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.17920 (11)	0.14364 (6)	0.056454 (19)	0.01599 (13)
O1	0.4150 (4)	0.24855 (18)	0.33907 (6)	0.0147 (3)
O2	−0.0788 (4)	−0.30118 (19)	0.30226 (6)	0.0175 (3)
O3	0.2039 (4)	−0.2523 (3)	0.49681 (6)	0.0257 (3)
C1	0.3352 (5)	0.0873 (3)	0.38908 (8)	0.0149 (4)
C2	0.1817 (5)	−0.1014 (3)	0.38028 (8)	0.0143 (4)
C3	0.0832 (5)	−0.1417 (3)	0.31299 (8)	0.0125 (3)
C4	0.1395 (4)	0.0114 (3)	0.19037 (8)	0.0124 (3)
C5	0.2401 (4)	0.1770 (3)	0.14057 (8)	0.0125 (3)
C6	0.3901 (4)	0.3707 (3)	0.15567 (8)	0.0123 (3)
C7	0.4419 (4)	0.3892 (3)	0.22300 (8)	0.0131 (3)
C8	0.1912 (4)	0.0316 (3)	0.25829 (8)	0.0117 (3)
C9	0.3461 (4)	0.2198 (3)	0.27341 (8)	0.0122 (3)
C10	0.4919 (5)	0.5510 (3)	0.10037 (9)	0.0158 (4)
C11	0.1133 (5)	−0.2676 (3)	0.43982 (9)	0.0185 (4)
H1	0.3904	0.1068	0.4340	0.0179*
H2	0.0357	−0.1156	0.1786	0.0149*
H3	0.5426	0.5171	0.2349	0.0157*
H4A	0.6025	0.6673	0.1203	0.0190*
H5B	0.2824	0.6139	0.0758	0.0190*

H6C	0.6571	0.4893	0.0690	0.0190*
H7	−0.0088	−0.3940	0.4331	0.0222*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0226 (3)	0.0153 (2)	0.0106 (2)	−0.00165 (14)	−0.00239 (13)	−0.00318 (13)
O1	0.0210 (6)	0.0146 (6)	0.0093 (6)	−0.0054 (5)	−0.0015 (5)	−0.0026 (4)
O2	0.0222 (7)	0.0151 (6)	0.0160 (6)	−0.0074 (5)	−0.0018 (5)	−0.0024 (5)
O3	0.0382 (8)	0.0262 (7)	0.0129 (7)	−0.0108 (6)	−0.0028 (6)	0.0009 (5)
C1	0.0178 (8)	0.0169 (8)	0.0102 (8)	−0.0016 (6)	−0.0000 (6)	−0.0019 (6)
C2	0.0161 (8)	0.0148 (8)	0.0121 (8)	−0.0014 (6)	0.0000 (6)	−0.0018 (6)
C3	0.0119 (7)	0.0129 (7)	0.0130 (8)	−0.0000 (6)	−0.0002 (6)	−0.0030 (6)
C4	0.0123 (8)	0.0113 (7)	0.0142 (8)	−0.0005 (6)	−0.0012 (6)	−0.0039 (6)
C5	0.0125 (8)	0.0140 (7)	0.0116 (7)	0.0012 (6)	−0.0012 (6)	−0.0037 (6)
C6	0.0101 (7)	0.0113 (7)	0.0151 (8)	0.0011 (6)	−0.0000 (6)	−0.0015 (6)
C7	0.0128 (8)	0.0108 (7)	0.0160 (8)	−0.0011 (6)	−0.0004 (6)	−0.0032 (6)
C8	0.0119 (8)	0.0110 (7)	0.0125 (8)	−0.0000 (6)	−0.0016 (6)	−0.0026 (6)
C9	0.0124 (8)	0.0136 (7)	0.0114 (8)	0.0001 (6)	−0.0017 (6)	−0.0044 (6)
C10	0.0198 (8)	0.0120 (7)	0.0152 (8)	−0.0021 (6)	0.0010 (6)	0.0001 (6)
C11	0.0237 (9)	0.0177 (8)	0.0143 (8)	−0.0054 (7)	−0.0004 (7)	−0.0015 (6)

Geometric parameters (Å, º)

Cl1—C5	1.7418 (19)	C6—C7	1.384 (3)
O1—C1	1.341 (3)	C6—C10	1.505 (3)
O1—C9	1.379 (3)	C7—C9	1.395 (3)
O2—C3	1.228 (3)	C8—C9	1.394 (3)
O3—C11	1.214 (3)	C1—H1	0.950
C1—C2	1.355 (3)	C4—H2	0.950
C2—C3	1.460 (3)	C7—H3	0.950
C2—C11	1.478 (3)	C10—H4A	0.980
C3—C8	1.477 (3)	C10—H5B	0.980
C4—C5	1.378 (3)	C10—H6C	0.980
C4—C8	1.398 (3)	C11—H7	0.950
C5—C6	1.414 (3)		
Cl1···C10	3.061 (5)	O3···H7^{iv}	3.3646
O1···C3	2.874 (5)	O3···H7^{viii}	2.5400
O2···C1	3.580 (5)	C1···H7^{ii}	3.5865
O2···C4	2.865 (4)	C2···H1^{vii}	3.4323
O2···C11	2.895 (3)	C2···H7^{iv}	3.5942
O3···C1	2.825 (4)	C3···H3^{v}	3.5438
C1···C7	3.584 (4)	C3···H3^{vi}	3.2093
C1···C8	2.751 (3)	C4···H2^{iv}	3.4855
C2···C9	2.772 (4)	C4···H3^{vi}	3.3323
C4···C7	2.797 (5)	C4···H4A^{v}	3.4637
C5···C9	2.742 (3)	C4···H4A^{vi}	3.1405

C6···C8	2.821 (4)	C4···H5B^{vi}	3.5800
Cl1···Cl1^{i}	3.397 (3)	C5···H2^{iv}	3.4899
O1···O2^{ii}	3.259 (5)	C5···H4A^{vi}	3.4169
O1···O2^{iii}	3.432 (5)	C5···H6C^{vii}	3.0939
O1···C2^{iv}	3.578 (6)	C6···H2^{ii}	3.4420
O1···C3^{iv}	3.487 (6)	C6···H4A^{vii}	3.4668
O2···O1^{v}	3.432 (5)	C6···H6C^{vii}	3.3186
O2···O1^{vi}	3.259 (5)	C7···H2^{ii}	3.3414
O2···C2^{vii}	3.452 (5)	C7···H3^{vii}	3.4983
O2···C3^{vii}	3.313 (6)	C8···H3^{vi}	3.4446
O2···C7^{v}	3.282 (4)	C9···H3^{vii}	3.5296
O2···C7^{vi}	3.222 (5)	C10···H2^{ii}	3.1715
O2···C8^{vii}	3.422 (6)	C10···H2^{iii}	3.5202
O2···C9^{vi}	3.389 (5)	C10···H4A^{vii}	3.4653
O3···O3^{viii}	3.462 (5)	C10···H5B^{iv}	3.0874
O3···O3^{ix}	3.400 (5)	C10···H6C^{vii}	3.3170
O3···C1^{ix}	3.271 (4)	C10···H6C^{xii}	3.4850
O3···C1^{x}	3.212 (4)	C11···H1^{vii}	3.4892
O3···C11^{viii}	3.306 (5)	C11···H1^{ix}	3.3664
C1···O3^{ix}	3.271 (4)	C11···H1^{x}	3.4654
C1···O3^{x}	3.212 (4)	C11···H7^{iv}	3.4101
C1···C2^{iv}	3.390 (6)	C11···H7^{viii}	3.0703
C1···C3^{iv}	3.530 (5)	H1···O3^{ix}	2.8065
C2···O1^{vii}	3.578 (6)	H1···O3^{x}	2.3848
C2···O2^{iv}	3.452 (5)	H1···C2^{iv}	3.4323
C2···C1^{vii}	3.390 (6)	H1···C11^{iv}	3.4892
C3···O1^{vii}	3.487 (6)	H1···C11^{ix}	3.3664
C3···O2^{iv}	3.313 (6)	H1···C11^{x}	3.4654
C3···C1^{vii}	3.530 (5)	H1···H1^{x}	2.8906
C3···C9^{vii}	3.522 (6)	H1···H7^{ii}	3.3381
C4···C6^{vii}	3.537 (6)	H2···C4^{vii}	3.4855
C4···C7^{vii}	3.548 (6)	H2···C5^{vii}	3.4899
C5···C6^{vii}	3.424 (6)	H2···C6^{vi}	3.4420
C5···C10^{vii}	3.599 (6)	H2···C7^{vi}	3.3414
C6···C4^{iv}	3.537 (6)	H2···C10^{v}	3.5202
C6···C5^{iv}	3.424 (6)	H2···C10^{vi}	3.1715
C7···O2^{ii}	3.222 (5)	H2···H3^{v}	3.0807
C7···O2^{iii}	3.282 (4)	H2···H3^{vi}	2.9969
C7···C4^{iv}	3.548 (6)	H2···H4A^{v}	2.5702
C7···C8^{iv}	3.533 (6)	H2···H4A^{vi}	2.8020
C8···O2^{iv}	3.422 (6)	H2···H5B^{vi}	2.9247
C8···C7^{vii}	3.533 (6)	H3···O2^{ii}	2.9512
C8···C9^{vii}	3.396 (6)	H3···O2^{iii}	2.4107
C9···O2^{ii}	3.389 (5)	H3···C3^{ii}	3.2093
C9···C3^{iv}	3.522 (6)	H3···C3^{iii}	3.5438
C9···C8^{iv}	3.396 (6)	H3···C4^{ii}	3.3323
C10···C5^{iv}	3.599 (6)	H3···C7^{iv}	3.4983
C11···O3^{viii}	3.306 (5)	H3···C8^{ii}	3.4446

C11···C11^{viii}	3.581 (5)	H3···C9^{iv}	3.5296
Cl1···H2	2.7736	H3···H2^{ii}	2.9969
Cl1···H5B	3.0008	H3···H2^{iii}	3.0807
Cl1···H6C	2.9039	H4A···Cl1^{ii}	3.3558
O1···H3	2.5156	H4A···C4^{ii}	3.1405
O2···H2	2.6042	H4A···C4^{iii}	3.4637
O2···H7	2.6084	H4A···C5^{ii}	3.4169
O3···H1	2.4980	H4A···C6^{iv}	3.4668
C1···H7	3.2820	H4A···C10^{iv}	3.4653
C3···H1	3.2957	H4A···H2^{ii}	2.8020
C3···H2	2.6739	H4A···H2^{iii}	2.5702
C3···H7	2.6867	H4A···H5B^{iv}	2.7486
C5···H3	3.2635	H5B···Cl1^{ii}	3.2097
C5···H4A	3.3351	H5B···Cl1^{xi}	3.3310
C5···H5B	2.8070	H5B···Cl1^{xii}	3.5195
C5···H6C	2.7698	H5B···C4^{ii}	3.5800
C6···H2	3.2984	H5B···C10^{vii}	3.0874
C7···H4A	2.5561	H5B···H2^{ii}	2.9247
C7···H5B	3.1190	H5B···H4A^{vii}	2.7486
C7···H6C	3.1491	H5B···H6C^{vii}	2.5591
C8···H3	3.2892	H5B···H6C^{xii}	3.0471
C9···H1	3.1874	H6C···Cl1^{iv}	2.8645
C9···H2	3.2616	H6C···Cl1^{xii}	3.1901
C10···H3	2.6736	H6C···C5^{iv}	3.0939
C11···H1	2.5574	H6C···C6^{iv}	3.3186
H1···H7	3.4925	H6C···C10^{iv}	3.3170
H3···H4A	2.3514	H6C···C10^{xii}	3.4850
H3···H5B	3.3096	H6C···H5B^{iv}	2.5591
H3···H6C	3.3584	H6C···H5B^{xii}	3.0471
Cl1···H4A^{vi}	3.3558	H6C···H6C^{xii}	3.0105
Cl1···H5B^{vi}	3.2097	H7···O1^{vi}	3.4049
Cl1···H5B^{xi}	3.3310	H7···O3^{vii}	3.3646
Cl1···H5B^{xii}	3.5195	H7···O3^{viii}	2.5400
Cl1···H6C^{vii}	2.8645	H7···C1^{vi}	3.5865
Cl1···H6C^{xii}	3.1901	H7···C2^{vii}	3.5942
O1···H7^{ii}	3.4049	H7···C11^{vii}	3.4101
O2···H3^{v}	2.4107	H7···C11^{viii}	3.0703
O2···H3^{vi}	2.9512	H7···H1^{vi}	3.3381
O3···H1^{ix}	2.8065	H7···H7^{viii}	2.7996
O3···H1^{x}	2.3848		

C1—O1—C9	118.32 (15)	O1—C9—C7	116.26 (16)
O1—C1—C2	124.81 (17)	O1—C9—C8	121.84 (15)
C1—C2—C3	120.85 (15)	C7—C9—C8	121.90 (17)
C1—C2—C11	119.27 (17)	O3—C11—C2	123.93 (18)
C3—C2—C11	119.87 (17)	O1—C1—H1	117.595
O2—C3—C2	123.93 (15)	C2—C1—H1	117.592
O2—C3—C8	122.62 (17)	C5—C4—H2	120.213

C2—C3—C8	113.45 (16)	C8—C4—H2	120.226
C5—C4—C8	119.56 (17)	C6—C7—H3	120.052
Cl1—C5—C4	118.24 (15)	C9—C7—H3	120.055
Cl1—C5—C6	119.54 (13)	C6—C10—H4A	109.463
C4—C5—C6	122.22 (17)	C6—C10—H5B	109.471
C5—C6—C7	117.93 (15)	C6—C10—H6C	109.471
C5—C6—C10	121.19 (17)	H4A—C10—H5B	109.473
C7—C6—C10	120.87 (16)	H4A—C10—H6C	109.475
C6—C7—C9	119.89 (17)	H5B—C10—H6C	109.474
C3—C8—C4	121.00 (16)	O3—C11—H7	118.044
C3—C8—C9	120.54 (16)	C2—C11—H7	118.029
C4—C8—C9	118.46 (15)		

C1—O1—C9—C7	−178.36 (12)	H2—C4—C5—C6	178.9
C1—O1—C9—C8	1.3 (2)	H2—C4—C8—C3	−0.6
C9—O1—C1—C2	−1.9 (3)	H2—C4—C8—C9	179.6
C9—O1—C1—H1	178.1	Cl1—C5—C6—C7	−178.56 (10)
O1—C1—C2—C3	−1.1 (3)	Cl1—C5—C6—C10	1.2 (2)
O1—C1—C2—C11	179.01 (13)	C4—C5—C6—C7	1.3 (3)
H1—C1—C2—C3	178.9	C4—C5—C6—C10	−178.89 (13)
H1—C1—C2—C11	−1.0	C5—C6—C7—C9	−0.1 (3)
C1—C2—C3—O2	−174.55 (15)	C5—C6—C7—H3	179.9
C1—C2—C3—C8	4.3 (2)	C5—C6—C10—H4A	−176.9
C1—C2—C11—O3	−4.2 (3)	C5—C6—C10—H5B	63.1
C1—C2—C11—H7	175.8	C5—C6—C10—H6C	−56.9
C3—C2—C11—O3	175.88 (15)	C7—C6—C10—H4A	2.8
C3—C2—C11—H7	−4.1	C7—C6—C10—H5B	−117.1
C11—C2—C3—O2	5.3 (3)	C7—C6—C10—H6C	122.8
C11—C2—C3—C8	−175.85 (13)	C10—C6—C7—C9	−179.90 (13)
O2—C3—C8—C4	−5.7 (3)	C10—C6—C7—H3	0.1
O2—C3—C8—C9	174.08 (14)	C6—C7—C9—O1	178.34 (13)
C2—C3—C8—C4	175.51 (13)	C6—C7—C9—C8	−1.3 (3)
C2—C3—C8—C9	−4.8 (2)	H3—C7—C9—O1	−1.7
C5—C4—C8—C3	179.37 (13)	H3—C7—C9—C8	178.7
C5—C4—C8—C9	−0.4 (3)	C3—C8—C9—O1	2.2 (3)
C8—C4—C5—Cl1	178.80 (12)	C3—C8—C9—C7	−178.17 (13)
C8—C4—C5—C6	−1.1 (3)	C4—C8—C9—O1	−178.08 (13)
H2—C4—C5—Cl1	−1.2	C4—C8—C9—C7	1.6 (3)

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) *x*, *y*+1, *z*; (iii) *x*+1, *y*+1, *z*; (iv) *x*+1, *y*, *z*; (v) *x*−1, *y*−1, *z*; (vi) *x*, *y*−1, *z*; (vii) *x*−1, *y*, *z*; (viii) −*x*, −*y*−1, −*z*+1; (ix) −*x*, −*y*, −*z*+1; (x) −*x*+1, −*y*, −*z*+1; (xi) −*x*, −*y*+1, −*z*; (xii) −*x*+1, −*y*+1, −*z*.